

A Novel Hyperbolization Procedure for the Two- Phase Six-Equation Flow Model

Samet Y. Kadioglu
Robert Nourgaliev
Nam Dinh

October 2011



The INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance

A Novel Hyperbolization Procedure for the Two-Phase Six-Equation Flow Model

**Samet Y. Kadioglu
Robert Nourgaliev
Nam Dinh**

October 2011

**Idaho National Laboratory
Idaho Falls, Idaho 83415**

<http://www.inl.gov>

**Prepared for the
U.S. Department of Energy
Through the INL LDRD Program
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517**

A Novel Hyperbolization Procedure for The Two-Phase Six-Equation Flow Model

Samet Y. Kadioglu

*Fuels Modeling and Simulation Department, Idaho National Laboratory, P.O. Box 1625,
MS 3840, Idaho Falls, ID 83415*

Robert Nourgaliev

*Reactor Physics Analysis and Design, Idaho National Laboratory, P. O. Box 1625, MS
3840, Idaho Falls, ID 83415*

Nam Dinh

*Reactor Physics Analysis and Design, Idaho National Laboratory, P. O. Box 1625, MS
3850, Idaho Falls, ID 83415*

Abstract

We introduce a novel approach for the hyperbolization of the well-known two-phase six-equation flow model. The six-equation model has been frequently used in many two-phase flow applications such as bubbly fluid flows in nuclear reactors. One major drawback of this model is that it can be arbitrarily non-hyperbolic resulting in difficulties such as numerical instability issues. Non-hyperbolic behavior can be associated with complex eigenvalues that correspond to characteristic matrix of the system. Complex eigenvalues are often due to certain flow parameter choices such as the definition of inter-facial pressure terms. In our method, we prevent the characteristic matrix receiving complex eigenvalues by fine tuning the inter-facial pressure terms with an iterative procedure. In this way, the characteristic matrix possesses all real eigenvalues meaning that the characteristic wave speeds are all real therefore the overall two-phase flow model becomes hyperbolic. The main advantage of this is that one can apply less diffusive highly accurate high resolution numerical schemes that often rely on explicit calculations of real eigenvalues. We note that existing non-hyperbolic models are discretized mainly based on low order highly dissipative numerical techniques in order to avoid stability issues.

Key words: Two-phase flow, Hyperbolicity, Six-equation model

Email addresses: Samet.Kadioglu@inl.gov (Samet Y. Kadioglu),
Robert.Nourgaliev@inl.gov (Robert Nourgaliev), Nam.Dinh@inl.gov
(Nam Dinh).

1 Governing Equations

Six-equation model for two-phase flows can be written as mass, momentum, and energy balances for each phases;

Phase-1:

$$\frac{\partial}{\partial t}[\alpha_1 \rho_1] + \frac{\partial}{\partial x}[\alpha_1 \rho_1 u_1] = 0, \quad (1)$$

$$\frac{\partial}{\partial t}[\alpha_1 \rho_1 u_1] + \frac{\partial}{\partial x}[\alpha_1 \rho_1 u_1^2 + \alpha_1 p] = p_I \frac{\partial \alpha_1}{\partial x}, \quad (2)$$

$$\frac{\partial}{\partial t}[\alpha_1 E_1] + \frac{\partial}{\partial x}[\alpha_1 (E_1 + p) u_1] = -p \left[\frac{\partial \alpha_1}{\partial t} + u_I \frac{\partial \alpha_1}{\partial x} \right] + u_I p_I \frac{\partial \alpha_1}{\partial x}, \quad (3)$$

Phase-2:

$$\frac{\partial}{\partial t}[\alpha_2 \rho_2] + \frac{\partial}{\partial x}[\alpha_2 \rho_2 u_2] = 0, \quad (4)$$

$$\frac{\partial}{\partial t}[\alpha_2 \rho_2 u_2] + \frac{\partial}{\partial x}[\alpha_2 \rho_2 u_2^2 + \alpha_2 p] = p_I \frac{\partial \alpha_2}{\partial x}, \quad (5)$$

$$\frac{\partial}{\partial t}[\alpha_2 E_2] + \frac{\partial}{\partial x}[\alpha_2 (E_2 + p) u_2] = -p \left[\frac{\partial \alpha_2}{\partial t} + u_I \frac{\partial \alpha_2}{\partial x} \right] + u_I p_I \frac{\partial \alpha_2}{\partial x}, \quad (6)$$

where α_i is the volume fraction of phase- i , ρ_i , u_i , and E_i are the density, velocity, and total energy of phase- i , p is the single pressure of the two-phase system, $p_I = p - \Delta p$ is referred to as the inter-facial pressure term with $\Delta p = \alpha_1 \rho_2 (u_1 - u_2)^2$, and $u_I = u_i$ for each phase (Theofanous *et al* ASME report [2]). Note : Saurel *et al* defines $u_I = \frac{\alpha_1 \rho_1 u_1 + \alpha_2 \rho_2 u_2}{\alpha_1 \rho_1 + \alpha_2 \rho_2}$ in their *seven-equation* model [3].

We can rewrite Eqs (1)-(6) in a more compact vector form by grouping mass, momentum, and energy terms for phase 1 and 2;

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = S, \quad (7)$$

where

$$U = \begin{pmatrix} \alpha_1 \rho_1 \\ \alpha_2 \rho_2 \\ \alpha_1 \rho_1 u_1 \\ \alpha_2 \rho_2 u_2 \\ \alpha_1 E_1 \\ \alpha_2 E_2 \end{pmatrix},$$

$$F = \begin{pmatrix} \alpha_1 \rho_1 u_1 \\ \alpha_2 \rho_2 u_2 \\ \alpha_1 \rho_1 u_1^2 + \alpha_1 p \\ \alpha_2 \rho_2 u_2^2 + \alpha_2 p \\ \alpha_1 (E_1 + p) u_1 \\ \alpha_2 (E_2 + p) u_2 \end{pmatrix},$$

$$S = \begin{pmatrix} 0 \\ 0 \\ p_I \frac{\partial \alpha_1}{\partial x} \\ p_I \frac{\partial \alpha_2}{\partial x} \\ -p \left[\frac{\partial \alpha_1}{\partial t} + u_I \frac{\partial \alpha_1}{\partial x} \right] + u_I p_I \frac{\partial \alpha_1}{\partial x} \\ -p \left[\frac{\partial \alpha_2}{\partial t} + u_I \frac{\partial \alpha_2}{\partial x} \right] + u_I p_I \frac{\partial \alpha_2}{\partial x} \end{pmatrix}.$$

If we introduce a vector $V = (\alpha_1, p, u_1, u_2, e_1, e_2)$ consisting of the primitive variables (e.g, $e_1 = (E_1 - 1/2 \rho_1 u_1^2)/\rho_1$) and recall that $\alpha_2 = 1 - \alpha_1$ and $c_i^2 = \left(\frac{\partial p}{\partial \rho_i} \right) |_{i=1,2}$, then (7) becomes

$$\frac{\partial U}{\partial V} \frac{\partial V}{\partial t} + \frac{\partial F}{\partial V} \frac{\partial V}{\partial x} = S^t \frac{\partial V}{\partial t} + S^x \frac{\partial V}{\partial x}, \quad (8)$$

where

$$\frac{\partial U}{\partial V} = \left(\frac{\partial u_i}{\partial v_j} \Big|_{i,j=1,2,3} \right),$$

$$\frac{\partial F}{\partial V} = \left(\frac{\partial f_i}{\partial v_j} \Big|_{i,j=1,2,3} \right)$$

are the Jacobian matrices of the transformation (refer to Table 1), and

$$S^t = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -p & 0 & 0 & 0 & 0 & 0 \\ p & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

Table 1. Jacobian matrices of the transformation used in (8).

$$\frac{\partial U}{\partial V} = \begin{pmatrix} \rho_1 & \frac{\alpha_1}{c_1^2} & 0 & 0 & 0 & 0 \\ -\rho_2 & \frac{(1-\alpha_1)}{c_2^2} & 0 & 0 & 0 & 0 \\ \rho_1 u_1 & \frac{\alpha_1 u_1}{c_1^2} & \alpha_1 \rho_1 & 0 & 0 & 0 \\ -\rho_2 u_2 & \frac{(1-\alpha_1)u_2}{c_2^2} & 0 & (1-\alpha_1)\rho_2 & 0 & 0 \\ \rho_1 e_1 + \frac{\rho_1 u_1^2}{2} & \frac{\alpha_1(e_1+1/2u_1^2)}{c_1^2} & \alpha_1 \rho_1 u_1 & 0 & \alpha_1 \rho_1 & 0 \\ -(\rho_2 e_2 + \frac{\rho_2 u_2^2}{2}) & \frac{(1-\alpha_1)(e_2+1/2u_2^2)}{c_2^2} & 0 & (1-\alpha_1)\rho_2 u_2 & 0 & (1-\alpha_1)\rho_2 \end{pmatrix}$$

$$\frac{\partial F}{\partial V} = \begin{pmatrix} \rho_1 u_1 & \frac{\alpha_1 u_1}{c_1^2} & \alpha_1 \rho_1 & 0 & 0 & 0 \\ -\rho_2 u_2 & \frac{(1-\alpha_1)u_2}{c_2^2} & 0 & (1-\alpha_1)\rho_2 & 0 & 0 \\ \rho_1 u_1^2 + p & \alpha_1(1 + \frac{u_1^2}{c_1^2}) & 2\alpha_1 \rho_1 u_1 & 0 & 0 & 0 \\ -(\rho_2 u_2^2 + p) & (1-\alpha_1)(1 + \frac{u_2^2}{c_2^2}) & 0 & 2(1-\alpha_1)\rho_2 u_2 & 0 & 0 \\ (\rho_1 e_1 + \frac{\rho_1 u_1^2}{2} + p)u_1 & \alpha_1 u_1(\frac{(e_1+1/2u_1^2)}{c_1^2} + 1) & \alpha_1(\rho_1 e_1 + \frac{3\rho_1 u_1^2}{2} + p) & 0 & \alpha_1 \rho_1 u_1 & 0 \\ -(\rho_2 e_2 + \frac{\rho_2 u_2^2}{2} + p)u_2 & (1-\alpha_1)u_2(\frac{(e_2+1/2u_2^2)}{c_2^2} + 1) & 0 & (1-\alpha_1)(\rho_2 e_2 + \frac{3\rho_2 u_2^2}{2} + p) & 0 & (1-\alpha_1)\rho_2 u_2 \end{pmatrix}$$

$$S^x = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ p_I & 0 & 0 & 0 & 0 & 0 \\ -p_I & 0 & 0 & 0 & 0 & 0 \\ -u_I(p - p_I) & 0 & 0 & 0 & 0 & 0 \\ u_I(p - p_I) & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

Grouping like terms together in (8), we have

$$\left(\frac{\partial U}{\partial V} - S^t\right) \frac{\partial V}{\partial t} + \left(\frac{\partial F}{\partial V} - S^x\right) \frac{\partial V}{\partial x} = 0, \quad (9)$$

Equivalently, (9) can be written as

$$\frac{\partial V}{\partial t} + A \frac{\partial V}{\partial x} = 0, \quad (10)$$

where $A = \left(\frac{\partial U}{\partial V} - S^t\right)^{-1} \left(\frac{\partial F}{\partial V} - S^x\right)$. From the hyperbolic theory, we know that the real eigenvalues of A correspond to characteristic wave speeds of the system. To find the eigenvalues of A , we have to find the roots of the following characteristic polynomial,

$$|A - \lambda I_6| = 0, \quad (11)$$

where I_6 is the 6×6 identity matrix. Notice from Table 2 that the matrix A has the following form

$$A = \begin{pmatrix} B & 0 & 0 \\ \cdots & u_1 & 0 \\ \cdots & 0 & u_2 \end{pmatrix},$$

meaning that the *two* immediate roots of (11) are $\lambda_1 = u_1$, $\lambda_2 = u_2$. Therefore the eigenvalue problem (11) reduces to finding the roots of the following quartic polynomial

$$P(\lambda) = |B - \lambda I_4| = 0. \quad (12)$$

We introduce the following identities:

$$c_m^2 = \frac{c_1^2 c_2^2 (\alpha_1 \rho_2 + (1 - \alpha_1) \rho_1)}{(1 - \alpha_1) c_1^2 \rho_1 + \alpha_1 c_2^2 \rho_2} \quad (\text{mixture sound speed}) \quad (13)$$

Table 2. Matrices used in (11) and (12).

$$A = \begin{pmatrix} \frac{(1-\alpha_1)c_1^2\rho_1u_1+\alpha_1c_2^2\rho_2u_2}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{(1-\alpha_1)\alpha_1(u_1-u_2)}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{(1-\alpha_1)\alpha_1c_1^2\rho_1}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{-(1-\alpha_1)\alpha_1c_2^2\rho_2}{\alpha_1c_2^2\rho_2+(1-\alpha_1)c_1^2\rho_1} & 0 & 0 \\ \frac{c_1^2c_2^2\rho_1\rho_2(u_1-u_2)}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{(1-\alpha_1)c_1^2\rho_1u_2+\alpha_1c_2^2\rho_2u_1}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{\alpha_1c_1^2c_2^2\rho_1\rho_2}{\alpha_1c_2^2\rho_2+(1-\alpha_1)c_1^2\rho_1} & \frac{(1-\alpha_1)c_1^2c_2^2\rho_1\rho_2}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & 0 & 0 \\ \frac{p-p_I}{\alpha_1\rho_1} & \frac{1}{\rho_1} & u_1 & 0 & 0 & 0 \\ \frac{-(p-p_I)}{(1-\alpha_1)\rho_2} & \frac{1}{\rho_2} & 0 & u_2 & 0 & 0 \\ \frac{c_2^2p\rho_2(u_1-u_2)}{\rho_1((1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2)} & -\frac{(1-\alpha_1)p(u_1-u_2)}{\rho_1((1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2)} & \frac{\alpha_1c_2^2p\rho_2}{\rho_1(\alpha_1c_2^2\rho_2+(1-\alpha_1)c_1^2\rho_1)} & \frac{(1-\alpha_1)c_2^2p\rho_2}{\rho_1((1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2)} & u_1 & 0 \\ \frac{c_1^2p\rho_1(u_1-u_2)}{\rho_2(\alpha_1c_2^2\rho_2+(1-\alpha_1)c_1^2\rho_1)} & \frac{\alpha_1p(u_1-u_2)}{\rho_2(\alpha_1c_2^2\rho_2+(1-\alpha_1)c_1^2\rho_1)} & \frac{\alpha_1c_1^2p\rho_1}{\rho_2(\alpha_1c_2^2\rho_2+(1-\alpha_1)c_1^2\rho_1)} & \frac{(1-\alpha_1)c_1^2p\rho_1}{\rho_2((1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2)} & 0 & u_2 \end{pmatrix}$$

$$B = \begin{pmatrix} \frac{(1-\alpha_1)c_1^2\rho_1u_1+\alpha_1c_2^2\rho_2u_2}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{(1-\alpha_1)\alpha_1(u_1-u_2)}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{(1-\alpha_1)\alpha_1c_1^2\rho_1}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{-(1-\alpha_1)\alpha_1c_2^2\rho_2}{\alpha_1c_2^2\rho_2+(1-\alpha_1)c_1^2\rho_1} \\ \frac{c_1^2c_2^2\rho_1\rho_2(u_1-u_2)}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{(1-\alpha_1)c_1^2\rho_1u_2+\alpha_1c_2^2\rho_2u_1}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} & \frac{\alpha_1c_1^2c_2^2\rho_1\rho_2}{\alpha_1c_2^2\rho_2+(1-\alpha_1)c_1^2\rho_1} & \frac{(1-\alpha_1)c_1^2c_2^2\rho_1\rho_2}{(1-\alpha_1)c_1^2\rho_1+\alpha_1c_2^2\rho_2} \\ \frac{p-p_I}{\alpha_1\rho_1} & \frac{1}{\rho_1} & u_1 & 0 \\ \frac{-(p-p_I)}{(1-\alpha_1)\rho_2} & \frac{1}{\rho_2} & 0 & u_2 \end{pmatrix}$$

$$\begin{aligned}
Y &= \frac{\lambda - (u_1 + u_2)/2}{c_m}, \\
M &= \frac{u_1 - u_2}{2c_m}, \\
K_a &= \frac{\alpha_1 \Delta p + (1 - \alpha_1)c_1^2 \rho_1}{(\alpha_1 \rho_2 + (1 - \alpha_1)\rho_1)c_1^2}, \\
K_b &= \frac{(1 - \alpha_1)\Delta p + \alpha_1 c_2^2 \rho_2}{(\alpha_1 \rho_2 + (1 - \alpha_1)\rho_1)c_2^2}, \\
K_c &= \frac{\Delta p}{(\alpha_1 \rho_2 + (1 - \alpha_1)\rho_1)c_m^2}.
\end{aligned} \tag{14}$$

Using (13) and (14) in (12), we obtain

$$(Y - M)^2(Y + M)^2 - K_a(Y - M)^2 - K_b(Y + M)^2 + K_c = 0. \tag{15}$$

This can further simplify to

$$Y^4 + \bar{p}Y^2 + \bar{q}Y + \bar{r} = 0, \tag{16}$$

where $\bar{p} = -2M^2 - K_a - K_b$, $\bar{q} = 2(K_a - K_b)M$, and $\bar{r} = M^4 + K_c - (K_a + K_b)M^2$. Notice that the coefficients of this quartic equation can be interpreted as they are functions of Δp (e.g, $\bar{p} = \bar{p}(\Delta p)$, $\bar{q} = \bar{q}(\Delta p)$, $\bar{r} = \bar{r}(\Delta p)$). In general, Eq. (16) can accept *four* real, *two* real and *one* complex pair, or *two* complex pair roots. We are interested in all real roots. In literature, number of criterions/conditions on these coefficients have been derived under which all four roots become real. A well known methodology is due to Abramowitz Stegun [1]. However, all-real-roots conditions can be several pages long complicated algebraic expressions that are not necessarily simple to implement in a computer code. In this paper, we iteratively perturb Δp up-to certain level where the equation accepts all real roots. Recall that $\Delta p = p - p_I$ can be viewed as the perturbed pressure field by some amount. Before going into details of our procedure, we would like to briefly remind ourselves the classic methodology of finding the general roots of a quartic equation. The procedure was first introduced by a famous mathematician Lodovico Ferrari in *fifteenth* century. His first observation was that if $\bar{q} = 0$, then we have a biquadratic equation that can be easily solved;

$$Y_{1,2,3,4} = \pm \sqrt{\frac{-\bar{p} \pm \sqrt{\bar{p}^2 - 4\bar{r}}}{2}}, \tag{17}$$

otherwise, the roots of the quartic equation can be related to the roots of the following depressed or resolvent cubic equation,

$$Z^3 + PZ + Q = 0, \tag{18}$$

where $P = -\frac{\bar{p}^2}{12} - \bar{r}$ and $Q = -\frac{\bar{p}^3}{108} + \frac{\bar{p}\bar{r}}{3} - \frac{\bar{q}^2}{8}$. A method for finding the roots of a cubic equation was introduced by Geralamo Cardano (L. Ferrari's mentor).

Cardano's method provides three roots for (18) as

$$Z_1 = u + v, Z_2 = -\frac{u+v}{2} + i\frac{u-v}{2}\sqrt{3}, Z_3 = -\frac{u+v}{2} - i\frac{u-v}{2}\sqrt{3}, \quad (19)$$

where

$$u = \sqrt[3]{-\frac{Q}{2} \pm \sqrt{\frac{Q^2}{4} + \frac{P^3}{27}}}, \quad v = \begin{cases} -\frac{P}{3u} & \text{if } u \neq 0 \\ -\sqrt[3]{Q} & \text{if } u = 0. \end{cases} \quad (20)$$

Then, the roots of the quartic equation become

$$Y_{1,2,3,4} = \frac{\pm_s \sqrt{\bar{p} + 2y} \pm_t \sqrt{-\left(3\bar{p} + 2y \pm_s \frac{2\bar{q}}{\sqrt{\bar{p} + 2y}}\right)}}{2}, \quad (21)$$

where $y = -\frac{5}{6}\bar{p} + Z$ (any of Z 's from (19) would be sufficient).

Below, we focus on our iterative procedure. Basically, we assume that the roots are written in general complex forms such as $Y_j = a_j + ib_j$, $j = 1, 2, 3, 4$, and we form a functional composing of imaginary parts of Y_j 's (e.g, $F = b_1^2 + b_2^2 + b_3^2 + b_4^2$). Note that this functional also can be interpreted as a function of Δp (e.g, $F = F(\Delta p)$). The objective is to change Δp iteratively until we satisfy $F = 0$. Clearly, this means that we obtain all real roots.

Outline of the algorithm :

Given ϵ

DO $k = 1, k_{max}$

Set $\Delta p_0 = p - k\epsilon p_I$, $\Delta p_1 = p$, $\Delta p_2 = p + k\epsilon p_I$

Call Golden Search Alg. to find minimum of F in the interval $I_{\Delta p} = [\Delta p_0, \Delta p_2]$

Golden Search routine returns F_{min} at $\Delta p_{min} \in I_{\Delta p}$

If $F_{min} = 0$, set $\Delta p = \Delta p_{min}$ (all real roots) go to 10

ENDDO

10 Set $\lambda_i = Y_i, i = 1, 2, 3, 4$

We have tested this algorithm for finding the real roots of arbitrary polynomials whose coefficients are functions of Δp . Our initial findings indicate that the algorithm is quite effective and always guaranties real roots upon the perturbation of the inter-facial pressure terms. When it is implemented to real two-phase flow system, this procedure has to be used at the beginning of each Riemann problem step which is the necessary part of the numerical fluxing procedure of the whole flow algorithm. With this procedure, since physically more accurate characteristics wave information is provided, more accurate and more stable numerical fluxes are calculated making the entire flow solver more accurate and more stable.

References

- [1] M. Abramowitz and I. A. Stegun. *Handbook of mathematical functions*. U.S. National Bureau of Standards, 1964.
- [2] T. Theofanous *et al.* Hyperbolicity, discontinuities, and numerics of the two-fluid model. *ASME report*.
- [3] R. Saurel and R. Abgrall. A multiphase godunov method for compressible multifluid and multiphase flows. *J. Comput. Phys.*, 150:425–467, 1999.